CLAIMS

What is claimed is:

1. A method of producing an Isotope Map for data from a mass spectometric injection of a biological sample comprising:

a) performing Noise reduction and Centroiding with a Noise Reduction Module on said data from a mass spectometric injection of a biological sample, and

b) generating an Isotope Map from the noise reduced and centroided data, thereby producing an Isotope Map.

2. The method of claim 1, wherein said biological sample is comprised of unlabeled biomolecules.

3. The method of claim 1, wherein said biological sample is comprised of underivatized biomolecules.

4. The method of claim 1, wherein said biological sample is comprised of biomolecules that are both unlabeled and underivatized.

5. The method of claim 1, wherein said biological sample is comprised of cleaved biomolecules.

6. The method of claim 5, wherein said biomolecules are cleaved with an enzyme.

7. The method of claim 6, wherein said enzyme is trypsin.

8. A method for producing a Peptide Map from an Isotope Map for data from a

mass spectometric injection of a biological sample comprising:

a) performing Peptide Detection on an Isotope Map with a Peptide Detection Module, and

b) generating a Peptide Map from the results of the peptide detection, thereby producing a Peptide Map.

9. A method for determining the functions to align Peptide Maps from a pair of Peptide Maps, each representing a mass spectrometric injection of a biological sample, comprising:

a) performing Peptide Map Alignment on a pair of Peptide Maps with a Peptide Map Alignment Module, and

b) determining a column offset between the pair of injections, and

c) determining a retention time transformation function between the pair of injections.

10. A method for Alignment of Peptide Maps from a pair of Peptide Maps, each representing a mass spectrometric injection of a biological sample, comprising performing Peptide Map Alignment on a pair of Peptide Maps with a Peptide Map Alignment Module, and thereby producing Aligned Peptide Maps.

11. A method of determining differentially and uniquely expressed biomolecules from a pair of mass spectrometric injections of biological samples, comprising:

a) producing Isotope Maps for the samples;

b) producing Peptide Maps from the Isotope Maps;

c) aligning the Peptide Maps, and

d) determining the differences between the aligned maps.

12. A method of matching biomolecules from an LC-MS injection to LC-MS-MS fragmentation spectra from comprising:

a) producing Isotope Maps for the injections;

b) producing Peptide Maps from the Isotope Maps;

c) aligning the Peptide Maps, and

d) determining the matching biomolecules.

13. A computer implemented method of producing an Isotope Map for data from a mass spectometric injection of a biological sample comprising:

a) inputting data from a mass spectometric injection of a biological sample, and performing Noise reduction and Centroiding with a Noise Reduction Module on said, and

b) generating an Isotope Map from the noise reduced and centroided data, thereby producing an Isotope Map.

14. The computer implemented method of claim 13, wherein said biological sample is comprised of unlabeled biomolecules.

15. The computer implemented method of claim 13, wherein said biological sample is comprised of underivatized biomolecules.

16. The computer implemented method of claim 13, wherein said biological sample is comprised of biomolecules that are both unlabeled and underivatized.

17. The computer implemented method of claim 13, wherein said biological sample is comprised of cleaved biomolecules.

18. The computer implemented method of claim 17, wherein said biomolecules are cleaved with an enzyme.

19. The computer implemented method of claim 18, wherein said enzyme is trypsin.

20. A computer implemented method for producing a Peptide Map from an Isotope Map for data from a mass spectometric injection of a biological sample comprising:

a) inputting an Isotope Map;

b) performing Peptide Detection on said Isotope Map with a Peptide Detection Module, and

c) generating a Peptide Map from the results of the peptide detection, thereby producing a Peptide Map.

21. A computer implemented method for determining the functions to align Peptide Maps from a pair of Peptide Maps, each representing a mass spectrometric injection of a biological sample, comprising:

a) inputting a pair of Peptide Maps;

b) performing Peptide Map Alignment on a pair of Peptide Maps with a Peptide Map Alignment Module;

c) determining a column offset between the pair of injections, and

d) determining a retention time transformation function between the pair of injections.

22. A computer implemented method for Alignment of Peptide Maps from a pair of Peptide Maps, each representing a mass spectrometric injection of a biological sample, comprising inputting a pair of Peptide Maps, performing Peptide Map Alignment on said pair of Peptide Maps with a Peptide Map Alignment Module, and thereby producing Aligned Peptide Maps.

23. A computer implemented method of determining differentially and uniquely expressed biomolecules from a pair of mass spectrometric injections of biological samples, comprising:

a) inputting data from said injections;

b) producing Isotope Maps for the samples;

c) producing Peptide Maps from the Isotope Maps;

d) aligning the Peptide Maps, and

e) determining the differences between the aligned maps.

24. A computer implemented method of matching biomolecules from an LC-MS injection to LC-MS-MS fragmentation spectra from comprising:

a) inputting data from said injections;

b) producing Isotope Maps for the injections;

c) producing Peptide Maps from the Isotope Maps;

d) aligning the Peptide Maps, and

e) determining the matching biomolecules.

25. A computer-readable memory having stored thereon a program for producing an Isotope Map for data from a mass spectometric injection of a biological sample comprising:

a) computer code that receives as input data from a mass spectometric injection of a biological sample, and performing Noise reduction and Centroiding with a Noise Reduction Module on said, and

b) and computer code that generates an Isotope Map from the noise reduced and centroided data, thereby producing an Isotope Map.

26. The computer-readable memory of claim 25, wherein said biological sample is comprised of unlabeled biomolecules.

27. The computer-readable memory of claim 25, wherein said biological sample is comprised of underivatized biomolecules.

28. The computer-readable memory of claim 25, wherein said biological sample is comprised of biomolecules that are both unlabeled and underivatized.

29. The computer-readable memory of claim 25, wherein said biological sample is comprised of cleaved biomolecules.

30. The computer-readable memory of claim 29, wherein said biomolecules are cleaved with an enzyme.

31. The computer-readable memory of claim 30, wherein said enzyme is trypsin.

32. A computer-readable memory having stored thereon a program for producing a Peptide Map from an Isotope Map for data from a mass spectometric injection of a biological sample comprising:

a) computer code that receives as input an Isotope Map;

b) computer code that performs Peptide Detection on said Isotope Map with a Peptide Detection Module, and

c) computer code that generates a Peptide Map from the results of the peptide detection, thereby producing a Peptide Map.

33. A computer-readable memory having stored thereon a program for determining the functions to align Peptide Maps from a pair of Peptide Maps, each representing a mass spectrometric injection of a biological sample, comprising:

a) computer code that receives as input a pair of Peptide Maps;

b) computer code that performs Peptide Map Alignment on a pair of Peptide Maps with a Peptide Map Alignment Module;

c) computer code that determines a column offset between the pair of injections, and

d) computer code that determines a retention time transformation function between the pair of injections.

34. A computer-readable memory having stored thereon a program for Alignment of Peptide Maps from a pair of Peptide Maps, each representing a mass spectrometric injection of a biological sample, comprising computer code that receives as input a pair of Peptide Maps, and computer code that performs Peptide Map Alignment on said pair of Peptide Maps with a Peptide Map Alignment Module, and thereby produces Aligned Peptide Maps.

35. A computer-readable memory having stored thereon a program for determining differentially and uniquely expressed biomolecules from a pair of mass spectrometric injections of biological samples, comprising:

a) computer code that receives as input data from said injections;

b) computer code that produces Isotope Maps for the samples;

c) computer code that produces Peptide Maps from the Isotope Maps;

d) computer code that aligns the Peptide Maps, and

e) computer code that determines the differences between the aligned maps.

36. A computer-readable memory having stored thereon a program for matching biomolecules

from an LC-MS injection to LC-MS-MS fragmentation spectra from comprising:

a) computer code that receives as input data from said injections;

b) computer code that produces Isotope Maps for the injections;

c) computer code that produces Peptide Maps from the Isotope Maps;

d) computer code that aligns the Peptide Maps, and

e) computer code that determines the matching biomolecules.

37. A computer system for producing an Isotope Map for data from a mass spectometric injection of a biological sample comprising a processor and a memory coupled to said processor, said memory encoding one or more programs, said one or more programs causing said processor to perform a method comprising:

a) computer code that receives as input data from a mass spectometric injection of a biological sample, and performing Noise reduction and Centroiding with a Noise Reduction Module on said, and

b) computer code that generates an Isotope Map from the noise reduced and centroided data, thereby producing an Isotope Map.

38. The computer system of claim 37, wherein said biological sample is comprised of unlabeled biomolecules.

39. The computer system of claim 37, wherein said biological sample is comprised of underivatized biomolecules.

40. The computer system of claim 37, wherein said biological sample is comprised of biomolecules that are both unlabeled and underivatized.

41. The computer system of claim 37, wherein said biological sample is comprised of cleaved biomolecules.

42. The computer system of claim 41, wherein said biomolecules are cleaved with an enzyme.

43. The computer system of claim 42, wherein said enzyme is trypsin.

44. A computer system for producing a Peptide Map from an Isotope Map for data from a mass spectometric injection of a biological sample comprising a processor and a memory coupled to said processor, said memory encoding one or more programs, said one or more programs causing said processor to perform a method comprising:

a) computer code that receives as input an Isotope Map;

b) computer code that performs Peptide Detection on said Isotope Map with a Peptide Detection Module, and

c) computer code that generates a Peptide Map from the results of the peptide detection, thereby producing a Peptide Map.

45. A computer system for determining the functions to align Peptide Maps from a pair of Peptide Maps, each representing a mass spectrometric injection of a biological sample, comprising a processor and a memory coupled to said processor, said memory encoding one or more programs, said one or more programs causing said processor to perform a method comprising:

a) computer code that receives as input a pair of Peptide Maps;

b) computer code that performs Peptide Map Alignment on a pair of Peptide Maps with a Peptide Map Alignment Module;

c) computer code that determines a column offset between the pair of injections, and

d) computer code that determines a retention time transformation function between the pair of injections.

46. A computer system for Alignment of Peptide Maps from a pair of Peptide Maps, each representing a mass spectrometric injection of a biological sample, comprising a processor and a memory coupled to said processor, said memory encoding one or more programs, said one or more programs causing said processor to perform a method comprising computer code that receives as input a pair of Peptide Maps, and computer code that performs Peptide Map Alignment on said pair of Peptide Maps with a Peptide Map Alignment Module, and thereby

produces Aligned Peptide Maps.

47. A computer system for determining differentially and uniquely expressed biomolecules from a pair of mass spectrometric injections of biological samples, comprising a processor and a memory coupled to said processor, said memory encoding one or more programs, said one or more programs causing said processor to perform a method comprising:

a) computer code that receives as input data from said injections;

b) computer code that produces Isotope Maps for the samples;

c) computer code that produces Peptide Maps from the Isotope Maps;

d) computer code that aligns the Peptide Maps, and

e) computer code that determines the differences between the aligned maps.

48. A computer system for matching biomolecules from an LC-MS injection to LC-MS-MS fragmentation spectra from comprising a processor and a memory coupled to said processor, said memory encoding one or more programs, said one or more programs causing said processor to perform a method comprising:

a) computer code that receives as input data from said injections;

b) computer code that produces Isotope Maps for the injections;

c) computer code that produces Peptide Maps from the Isotope Maps;

d) computer code that aligns the Peptide Maps, and

e) computer code that determines the matching biomolecules.

49. A method for displaying information on an Isotope Map for data from a mass spectometric injection of a biological sample comprising:

a) inputting data from a mass spectometric injection of a biological sample;

b) performing Noise reduction and Centroiding with a Noise Reduction Module on said data;

b) generating an Isotope Map from the noise reduced and centroided data, thereby producing an Isotope Map, and

c) displaying information on said Isotope Map to a user..

50. The method of claim 49, wherein said biological sample is comprised of unlabeled biomolecules.

51. The method of claim 49, wherein said biological sample is comprised of underivatized biomolecules.

52. The method of claim 49, wherein said biological sample is comprised of biomolecules that are both unlabeled and underivatized.

53. The method of claim 49, wherein said biological sample is comprised of cleaved biomolecules.

54. The method of claim 53, wherein said biomolecules are cleaved with an enzyme.

55. The method of claim 54, wherein said enzyme is trypsin.

56. A method for displaying information on a Peptide Map produced from an Isotope Map for data from a mass spectometric injection of a biological sample comprising:

a) inputting an Isotope Map;

b) performing Peptide Detection on said Isotope Map with a Peptide Detection Module;

c) generating a Peptide Map from the results of the peptide detection, thereby producing a Peptide Map, and

d) displaying information on said Peptide Map to a user.

57. A method for displaying information on the functions to align Peptide Maps from a pair of Peptide Maps, each representing a mass spectrometric injection of a biological sample, comprising:

a) inputting a pair of Peptide Maps;

b) performing Peptide Map Alignment on a pair of Peptide Maps with

a Peptide Map Alignment Module;

c) determining a column offset between the pair of injections;

d) determining a retention time transformation function between the pair of injections, and

e) displaying information on said functions to a user.

58. A method for displaying information on Alignment of Peptide Maps from a pair of Peptide Maps, each representing a mass spectrometric injection of a biological sample, comprising inputting a pair of Peptide Maps, and performing Peptide Map Alignment on said pair of Peptide Maps with a Peptide Map Alignment Module, thereby producing Aligned Peptide Maps, displaying information on said Aligned Peptide Maps to a user.

59. A method for displaying information on differentially and uniquely expressed biomolecules from a pair of mass spectrometric injections of biological samples, comprising:

a) inputting data from said injections;

b) producing Isotope Maps for the samples;

c) producing Peptide Maps from the Isotope Maps;

d) aligning the Peptide Maps;

e) determining the differences between the aligned maps, and

f) displaying information on said differences to a user.

60. A method for displaying information on matching biomolecules from an LC-MS injection to LC-MS-MS fragmentation spectra from comprising:

a) inputting data from said injections;

b) producing Isotope Maps for the injections;

c) producing Peptide Maps from the Isotope Maps;

d) aligning the Peptide Maps, and

e) determining the matching biomolecules,

f) and displaying information on said matching biomolecules to a user.